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An Extreme-Scale Multi-Fidelity Computational Active Learning Paradigm Towards Realizing Autonomous Synthesis

Traditional approaches to bridge atomistic dynamics with experimental observations at the microstructural level often rely on phenomenological models of the underlying physics, whose free parameters are in turn fitted to a small number of intuition-driven atomic scale simulations under limited number of thermodynamical drivers (e.g., temperature, pressure, chemical potential etc). This tedious and time-consuming approach becomes particularly cumbersome to study synthesis of chemicals and materials with complex dependencies on local environment, temperature and lattice-strains e.g., heterostructure interfaces of nanomaterials. In this talk, I will present workflows that couple automated exascale high-throughput large-scale DFT calculations, ensemble force-field fitting and molecular dynamics simulations with a wide range of uncertainty quantification-driven active learning paradigms for on-the-fly learning of material synthesis trajectories, to create an autonomous computational synthesis platform. By implementing such a workflow to study recrystallization of amorphous transition-metal dichalcogenide (TMDC) phases under various growth parameters, I will show that such automated multi-fidelity frameworks can be promising towards achieving controlled epitaxy of targeted multilayer moiré devices paving the way towards a robust autonoumous discovery pipeline to enable unprecedented functionalities. Opportunities to use these autonomous computational synthesis pipelines to create 'digital twins' of synthesis trajectories, train generative inverse-design machine-learning algorithms to predict new materials and their synthesis parameters with targeted properties, and eventually accelarate experimental synthesis will also be presented.

Topical Area

AI and data science

Authors: GANESH, Panchapakesan (Oak Ridge National Laboratory); BAGCHI, Soumendu (Oak Ridge National Laboratory); MORELOCK, Ryan (Oak Ridge National Lab); FUHR, Addis; GHOSH, Ayana (Oak Ridge National Laboratory); MUKHERJEE, Debangshu; MAIER, Thomas

Presenter: GANESH, Panchapakesan (Oak Ridge National Laboratory)